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Electron-Impact Ionization Cross-Sections and Ionization Rate Coefficients for Atoms and Ions from Hydrogen to Calcium*

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Using the empirical formula recently proposed, electron-impact ionization cross-sections for single ionization from the ground state are given for free atoms and for all ionization stages from hydrogen to calcium ($Z=20$). Ionization rate coefficients are given for these species on the assumption of a Maxwellian distribution of the impacting electrons. Multiple ionization, lowering of ionization potential, or collision limit are not taken into account.

I. Introduction

In a recent paper, the author attempted to predict ionization cross-sections hitherto unknown in the triangle H I–Na I–Na XI on an empirical basis[1], after certain regularities had been discovered. In the meantime, the author has proposed an empirical formula with the help of which all experimentally determined cross-section curves can be approximated within the experimental error[2], and, in most cases, even within 10% over the whole energy range from threshold to 10 keV. With this formula it should be possible to extend the predictions as far as calcium and give better approximations for the elements beryllium through sodium.

II. The Formula Used

For predictions, Formula (4) of Ref. 2 is the most versatile and is used here:

$$\sigma = \sum_{i=1}^{N} a_i q_i \frac{\ln(E/P_i)}{E P_i} \{1 - b_i \exp[-c_i(E/P_i - 1)]\}; \quad E \geqq P_i. \qquad (1)$$

E is the energy of the impact electron; P_i is the binding energy of electrons in the i-th subshell; P_1 is the ionization potential; q_i is the number of equivalent electrons in the i-th subshell; a_i, b_i, and c_i are individual constants, which have to be determined by experiment, theory, or

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1 LOTZ, W.: Astrophys. J., Suppl. **14**, 207 (1967).
2 LOTZ, W.: Z. Physik **206**, 205 (1967).

reasonable guesswork. N is equal to 1 for hydrogen-like and helium-like ions; N is equal to 2 for lithium-like and beryllium-like ions; N is set equal to 2 for boron-like through neon-like ions, because here the contribution from the K shell is negligible; N is set equal to 3 for sodium-like through calcium-like ions in order to get a better approximation at the high energy tail of the cross-section curve. No distinction is made between the L_{II} and the L_{III} shells, it is assumed that all $2p$ electrons are equivalent and thus form one subshell. The same statement holds for $3p$ electrons in the M_{II} and M_{III} shells.

Near threshold $E \approx P_1$, Formula (1) reduces to

$$\sigma \approx a_1 q_1 \frac{E/P_1 - 1}{P_1^2} (1 - b_1) \propto U - 1, \tag{2}$$

with $U = E/P_1$. For large electron energies $E \gg P_i$, Formula (1) becomes

$$\sigma_i \approx a_i q_i \frac{\ln(E/P_i)}{E P_i} \propto \frac{\ln E}{E}. \tag{3}$$

Formula (1) thus gives the correct energy dependence both for small and for large energies of the impact electron.

In Tables 1 and 2 all quantities (except binding energies) needed for Formula (1) are tabulated for the first few ionization stages of hydrogen through calcium. Experimentally known are: H I, He I, He II, Li I, Li II, N I, N II, O I, Ne I, Ne II, Na I, Na II, A I, K I, and K II. The cross-sections of these species can be approximated with Formula (1) within the experimental error and, mostly, even within 10% over the whole energy range between threshold and 10 keV electron energy, similar to Ref. 2.

For the species not mentioned in Tables 1 or 2 (four times and higher ionized ions) I assumed that $a_i = 4.5 \times 10^{-14}$ cm^2 (eV)^2 and that $b_i = 0$. This assumption agrees within a few percent with the theoretical calculations of RUDGE and SCHWARTZ[3] for a hydrogen-like ion with high Z-number in the Born exchange approximation, and within 20% for a magnesium-like and a sodium-like ion with high Z-number (Fe XV and Fe XVI respectively) in the same approximation[4]. The validity of this assumption, especially for neon-like ions, might be questioned, but no better approximation is known.

The ionization potential of electrons in the outermost subshell[5], the binding energy of electrons in the next inner subshell[6], and the binding

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[3] RUDGE, M.R.H., and S.B. SCHWARTZ: Proc. Phys. Soc. (London) **88**, 563 (1966).
[4] RUDGE, M.R.H., and S.B. SCHWARTZ: Proc. Phys. Soc. (London) **88**, 579 (1966).
[5] LOTZ, W.: J. Opt. Soc. Am. **57**, 873 (1967).
[6] LOTZ, W.: J. Opt. Soc. Am. **58**, 236 (1968).

Table 1. *Relevant data for the first and the second ionization stage of the elements under consideration. a_i is given in 10^{-14} cm^2 (eV)^2*

Conf.	q_1	q_2	q_3	Species	a_1	a_2	a_3	b_1	b_2	b_3	c_1	c_2	c_3	Species	a_1	a_2	a_3	b_1	b_2	b_3	c_1	c_2	c_3
$1s$	1	0	0	H I	4.0	–	–	0.60	–	–	0.56	–	–	He II	4.4	–	–	0.38	–	–	0.60	–	–
$1s^2$	2	0	0	He I	4.0	–	–	0.75	–	–	0.46	–	–	Li II	4.0	–	–	0.48	–	–	0.60	–	–
$2s$	1	2	0	Li I	4.0	4.2	–	0.70	0.6	–	2.4	0.6	–	Be II	4.4	4.4	–	0	0.4	–	–	0.6	–
$2s^2$	2	2	0	Be I	4.0	4.2	–	0.7	0.6	–	0.5	0.6	–	B II	4.4	4.4	–	0.4	0.4	–	0.6	0.6	–
$2p$	1	2	0	B I	3.8	4.0	–	0.7	0.7	–	0.4	0.5	–	C II	4.2	4.4	–	0.4	0.4	–	0.6	0.6	–
$2p^2$	2	2	0	C I	3.5	4.0	–	0.7	0.7	–	0.4	0.5	–	N II	3.9	4.4	–	0.46	0.4	–	0.62	0.6	–
$2p^3$	3	2	0	N I	3.2	4.0	–	0.83	0.7	–	0.22	0.5	–	O II	3.7	4.4	–	0.6	0.4	–	0.6	0.6	–
$2p^4$	4	2	0	O I	2.8	4.0	–	0.74	0.7	–	0.24	0.5	–	F II	3.5	4.4	–	0.7	0.4	–	0.5	0.6	–
$2p^5$	5	2	0	F I	2.7	4.0	–	0.9	0.7	–	0.2	0.5	–	Ne II	3.2	4.4	–	0.83	0.4	–	0.48	0.6	–
$2p^6$	6	2	0	Ne I	2.6	4.0	–	0.92	0.7	–	0.19	0.5	–	Na II	3.4	4.4	–	0.84	0.4	–	0.32	0.6	–
$3s$	1	6	2	Na I	4.0	3.0	4.0	0	0.9	0.7	–	0.2	0.5	Mg II	4.4	3.7	4.4	0	0.8	0.4	–	0.4	0.6
$3s^2$	2	6	2	Mg I	4.0	3.0	4.0	0.4	0.9	0.7	0.6	0.2	0.5	Al II	4.4	3.7	4.4	0.2	0.8	0.4	0.6	0.4	0.6
$3p$	1	2	6	Al I	4.0	4.0	3.0	0.3	0.4	0.9	0.6	0.6	0.2	Si II	4.4	4.4	3.7	0.2	0.2	0.8	0.6	0.6	0.4
$3p^2$	2	2	6	Si I	4.0	4.0	3.0	0.3	0.4	0.9	0.6	0.6	0.2	P II	4.4	4.4	3.7	0.2	0.2	0.8	0.6	0.6	0.4
$3p^3$	3	2	6	P I	4.0	4.0	3.0	0.4	0.4	0.9	0.6	0.6	0.2	S II	4.4	4.4	3.7	0.3	0.2	0.8	0.6	0.6	0.4
$3p^4$	4	2	6	S I	4.0	4.0	3.0	0.4	0.4	0.9	0.6	0.6	0.2	Cl II	4.4	4.4	3.7	0.3	0.2	0.8	0.6	0.6	0.4
$3p^5$	5	2	6	Cl I	4.0	4.0	3.0	0.5	0.4	0.9	0.5	0.6	0.2	A II	4.2	4.4	3.7	0.3	0.2	0.8	0.6	0.6	0.4
$3p^6$	6	2	6	A I	4.0	4.0	3.0	0.62	0.4	0.9	0.40	0.6	0.2	K II	4.0	4.4	3.7	0.3	0.2	0.8	0.6	0.6	0.4
$4s$	1	6	2	K I	4.0	4.0	4.0	0	0.6	0.4	–	0.4	0.6	Ca II	4.4	4.4	4.4	0	0.3	0.2	–	0.6	0.6
$4s^2$	2	6	2	Ca I	4.0	4.0	4.0	0.4	0.6	0.4	0.6	0.4	0.6	–	–	–	–	–	–	–	–	–	–

energy of electrons in the second next inner subshell[7] have been taken from recent papers of the author.

[7] Lotz, W.: J. Opt. Soc. Am. **58**, 915 (1968).

Table 2. *Relevant data for the third and fourth ionization stage of the elements under consideration. a_i is given in 10^{-14} cm^2 (eV)^2*

Conf.	q_1	q_2	q_3	Species	a_1	a_2	a_3	b_1	b_2	b_3	c_1	c_2	c_3	Species	a_1	a_2	a_3	b_1	b_2	b_3	c_1	c_2	c_3
1s	1	0	0	Li III	4.5	–	–	0.2	–	–	0.6	–	–	Be IV	4.5	–	–	0	–	–	–	–	–
1s^2	2	0	0	Be III	4.5	–	–	0.3	–	–	0.6	–	–	B IV	4.5	–	–	0	–	–	–	–	–
2s	1	2	0	B III	4.5	4.5	–	0	0.2	–	–	0.6	–	C IV	4.5	4.5	–	0	0	–	–	–	–
2s^2	2	2	0	C III	4.5	4.5	–	0.2	0.2	–	0.6	0.6	–	N IV	4.5	4.5	–	0	0	–	–	–	–
2p	1	2	0	N III	4.5	4.5	–	0.2	0.2	–	0.6	0.6	–	O IV	4.5	4.5	–	0	0	–	–	–	–
2p^2	2	2	0	O III	4.5	4.5	–	0.3	0.2	–	0.6	0.6	–	F IV	4.5	4.5	–	0	0	–	–	–	–
2p^3	3	2	0	F III	4.5	4.5	–	0.4	0.2	–	0.6	0.6	–	Ne IV	4.5	4.5	–	0.2	0	–	0.6	–	–
2p^4	4	2	0	Ne III	4.2	4.5	–	0.5	0.2	–	0.6	0.6	–	Na IV	4.5	4.5	–	0.2	0	–	0.6	–	–
2p^5	5	2	0	Na III	4.0	4.5	–	0.6	0.2	–	0.5	0.6	–	Mg IV	4.5	4.5	–	0.3	0	–	0.6	–	–
2p^6	6	2	0	Mg III	4.0	4.5	–	0.6	0.2	–	0.5	0.6	–	Al IV	4.5	4.5	–	0.3	0	–	0.6	–	–
3s	1	6	2	Al III	4.5	4.2	4.5	0	0.6	0.2	–	0.5	0.6	Si IV	4.5	4.5	4.5	0	0.3	0	–	0.6	–
3s^2	2	6	2	Si III	4.5	4.2	4.5	0	0.6	0.2	–	0.5	0.6	P IV	4.5	4.5	4.5	0	0.3	0	–	0.6	–
3p	1	2	6	P III	4.5	4.5	4.2	0	0	0.6	–	–	0.5	S IV	4.5	4.5	4.5	0	0	0.3	–	–	0.6
3p^2	2	2	6	S III	4.5	4.5	4.2	0	0	0.6	–	–	0.5	Cl IV	4.5	4.5	4.5	0	0	0.3	–	–	0.6
3p^3	3	2	6	Cl III	4.5	4.5	4.2	0.2	0	0.6	0.6	–	0.5	A IV	4.5	4.5	4.5	0	0	0.3	–	–	0.6
3p^4	4	2	6	A III	4.5	4.5	4.2	0.2	0	0.6	0.6	–	0.5	K IV	4.5	4.5	4.5	0	0	0.3	–	–	0.6
3p^5	5	2	6	K III	4.5	4.5	4.2	0.2	0	0.6	0.6	–	0.5	Ca IV	4.5	4.5	4.5	0	0	0.3	–	–	0.6
3p^6	6	2	6	Ca III	4.5	4.5	4.2	0.2	0	0.6	0.6	–	0.5	Sc IV	4.5	4.5	4.5	0	0	0.3	–	–	0.6

III. Cross-Sections and Rate Coefficients

Cross-section curves for free atoms have been drawn with the data of Table 1 (Figs. 1 through 3). I estimate the error of these cross-sections to be not higher than $^{+40}_{-30}$% (twice the probable error). For cross-sections of atoms known experimentally, the respective curves can be found in earlier papers of the author[1,2]. The cross-sections of Fig. 1 are

different from those of Ref. 1, though they are within the stated error limits. The cross-section curve for sodium (Fig. 2) is appreciably lower than the experimental curve given in Ref. 1. As this is the only discrepancy

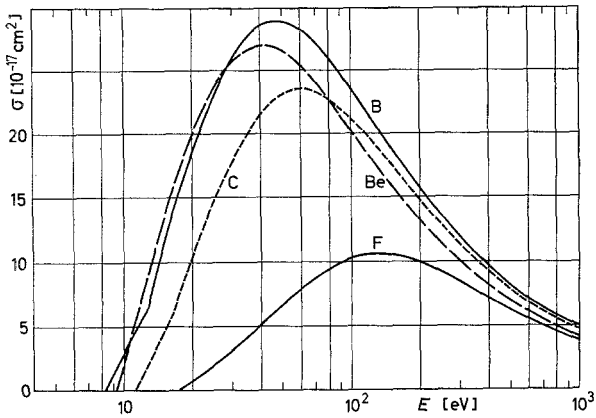

Fig. 1. Electron-impact ionization cross-sections for single ionization from the ground state of atomic beryllium, boron, carbon, and fluorine. Formula (1) and the data of Table 1 have been used

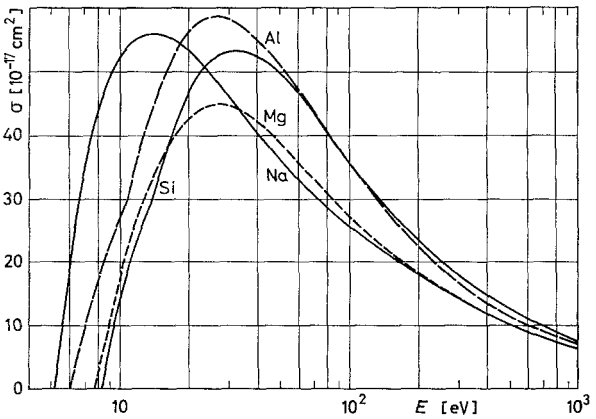

Fig. 2. Electron-impact ionization cross-sections for single ionization from the ground state of atomic sodium, magnesium, aluminum, and silicon. Formula (1) and the data of Table 1 have been used

with respect to experiments, I tend to place more confidence in the values of Fig. 2 than in the experimental values of sodium in Ref. 1.

Formula (1) can be folded with a Maxwellian electron distribution of temperature T

$$\frac{dn}{n}=\frac{2}{kT}\left(\frac{E}{\pi kT}\right)^{\frac{1}{2}}\exp(-E/kT)\,dE \tag{4}$$

and yields the following rate coefficient (in $cm^3\ s^{-1}$):

$$S = 6.7 \times 10^{-7} \sum_{i=1}^{N} \frac{a_i q_i}{T^{\frac{3}{2}}} \left\{ \frac{1}{P_i/T} \int_{P_i/T}^{\infty} \frac{e^{-x}}{x} dx - \frac{b_i \exp c_i}{P_i/T + c_i} \int_{P_i/T+c_i}^{\infty} \frac{e^{-y}}{y} dy \right\}, \quad (5)$$

when a_i is given in $10^{-14}\ cm^2\ (eV)^2$, and P_i and T in eV. These rate coefficients have been computed[8] with the data of Tables 1 and 2 for a

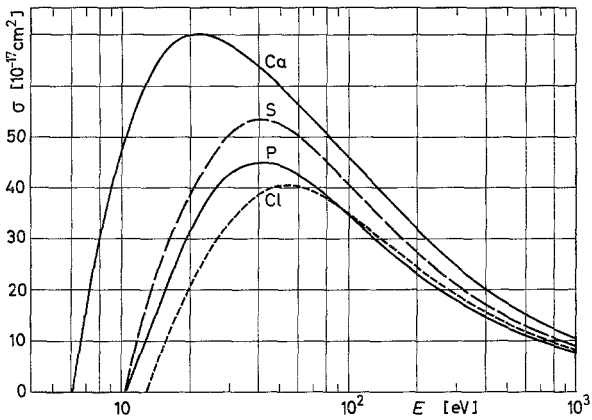

Fig. 3. Electron-impact ionization cross-sections for single ionization from the ground state of atomic phosphorus, sulfur, chlorine, and calcium. Formula (1) and the data of Table 1 have been used

number of discrete electron temperatures T between 1 and 10^4 eV and are given numerically in Ref.[8]. For oxygen these rate coefficients are given graphically in Fig. 4.

Fig. 1–3 give cross-sections of free atoms in their ground state for single ionization by electron impact. The rate coefficients of Ref.[8] and Fig. 4 might be too low for the following reasons:

(1) Multiple ionization,

(2) Lowering of ionization potential[9],

(3) A "collision limit" lower than the ionization potential, i.e. ionization from excited levels[10,11]

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[8] LOTZ, W.: Report IPP 1/62, Institut für Plasmaphysik, Garching bei München, 1967. This report contains 40 figures and the computed values not reproduced here. Reports are available on request from the author.

[9] STEWART, J.C., and K.D. PYATT: Astrophys. J. **144**, 1203 (1966).

[10] BATES, D.R., A.E. KINGSTON, and R.W.P. MCWHIRTER: Proc. Roy. Soc. (London) A **267**, 297 (1962).

[11] GRIEM, H.R.: In: Plasma Spectroscopy, p. 159. New York: McGraw-Hill Book Co. 1964.

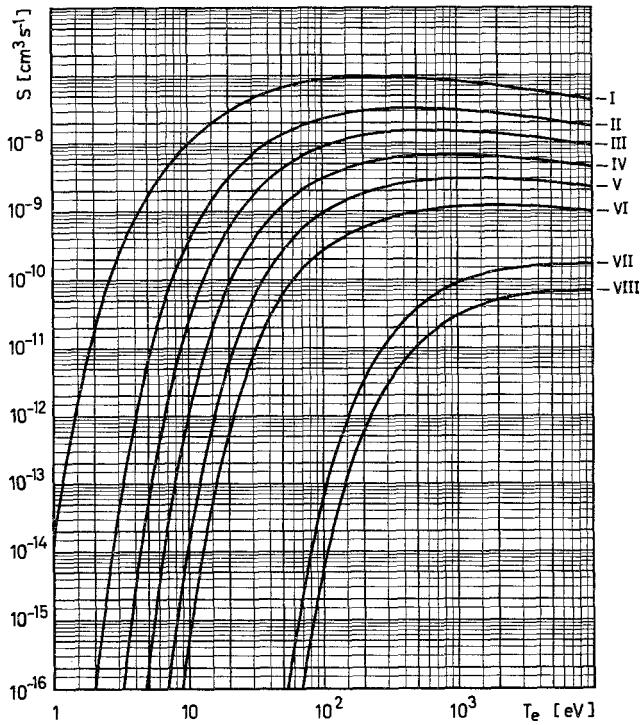

Fig. 4. Ionization rate coefficients for single ionization of oxygen atoms and ions from the ground state by electron-impact in a tenuous plasma (Maxwellian distribution, no lowering of ionization potential, no collision limit)

In cases (2) and (3) the ionization potential of Ref.[5] is to be replaced by the lowered ionization potential or by the value of the collision limit. It should still be possible then to use Formulae (1) and (5) after these corrections to the ionization potential have been applied, though the form of the cross-section curve might be changed drastically near threshold.

As the lowering of the ionization potential and the collision limit depend on electron density, the values given in Ref.[8] and Fig. 4 are asymptotically correct only for low densities (allowing for multiple ionization). For electron temperatures small compared with the ionization potential, the deviation to be expected for "higher" densities may be as large as an order of magnitude or more.

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